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EXCITED-STATE ENERGISTICS AND DYNAMICS OF LARGE
MOLECULES COMPLEXES AND CL. (U) TEL-AVIV UNIV (ISRAEL)
DEPT OF CHEMISTRY J JORTNER ET AL. APR 85

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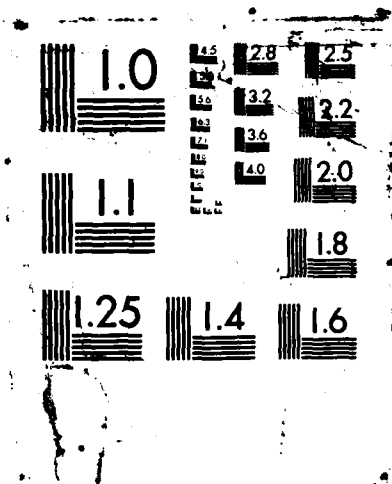
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FIRST INTERIM REPORT

Contract No. DAJA45-85-C-0008

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PROGRESS REPORT FOR THE PERIOD FEBRUARY - APRIL, 1985

1st Periodic Report

1. Title: EXCITED-STATE ENERGETICS AND DYNAMICS
OF LARGE MOLECULES, COMPLEXES AND
CLUSTERS
2. Principal Investigator: Professor Joshua Jortner
3. Associated Investigator: Professor Uzi Even
4. Contractor: The Department of Chemistry
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5. Contract No. DAJA45-85-C-0008

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6. PROGRESS IN TECHNICAL APPROACH

⇒ Vacuum Ultraviolet Absorption Spectroscopy in Supersonic Expansions. We have combined the techniques of vacuum ultraviolet (VUV) spectroscopy together with planar supersonic jets, which allows for the interrogation of absorption spectra of large molecules cooled in supersonic expansions in the near VUV region. The experimental setup consists of a high pressure Xe lamp, ^{vacuum} optics, a vacuum ultraviolet spectrograph and a nozzle slit (0.27x90 mm, repetition rate 9 Hz and gas pulse duration 300 μ sec). The characteristics of this spectroscopic setup are: (i) Energy range 6-10 eV. (ii) Spectral resolution 0.1 Å. (iii) Routine measurements of high-energy absorption spectra. (iv) Interrogation of fluorescence excitation spectra of the parent molecule or its photoproducts with limiting quantum yields of $Y \geq 10^{-4}$.

7. ACCOMPLISHMENTS OF OBJECTIVES

- 7.A Energetics of Rydberg States of Jet Cooled Molecules. VUV absorption spectra of benzene, benzene-D₆ and naphthalene cooled in planar supersonic expansions were measured over the range 2000-1600 Å, providing evidence on energetics, line broadening and interference effects.
- 7.B Intramolecular Relaxation of Rydberg States. Information on intramolecular dynamics of extravalence excitations of benzene was obtained from lineshape analysis. The lineshape of the ³P_{xy}(0) Rydberg is Lorentzian, whose homogeneous width result in the lifetime $\tau = 0.19 \pm 0.02$ psec for C₆H₆ and $\tau = 0.22 \pm 0.02$ psec for C₆D₆, implying that (i) the relaxation of the Rydberg is characterized by moderate energy gaps, and (ii) the electronic relaxation rate of the Rydberg is considerably less efficient than that of the intravalence excitation in the same energy domain.

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8. PUBLICATIONS

- (1) A. Amirav and J. Jortner
Vacuum Ultraviolet Absorption Spectroscopy in
Supersonic Expansions
J. Chem. Phys. (Communication) (in press)
- (2) U. Even, Z. Berkovitch-Yellin and J. Jortner
Electronic Excitations of the Free-Base Porphine-
Ar van der Waals Complex
Canad. J. Chem. (C. Sandorfy-Special Issue) (in press)

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